C. William McCurdy

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Professor of Applied Science, UC Davis; Adjunct Professor of Chemistry, UC Berkeley; CSD Senior Faculty Scientist; Atomic, Molecular and Optical Sciences (AMOS) Program

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Programs:
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Biography:
Adjunct Professor, born 1949; B.S.Tulane University (1971); Ph.D. Chemistry, California Institute of Technology (1976); Camille and Henry Dreyfus Teacher-Scholar Award (1982); Alfred P. Sloan Research Fellow (1981-1983); Ohio State University Distinguished Scholar Award (1984); Fellow of the American Physical Society (1993); Associate Laboratory Director for Computing Sciences, Lawrence Berkeley National Laboratory; Professor of Applied Science, University of California, Davis.

Research Interests:

Collisions of electrons and photons with molecules are being investigated with new theoretical techniques and parallel computing algorithms

Electron-molecule and electron-atom collisions initiate and drive almost all the relevant chemical processes associated with radiation chemistry in the environment, radiation damage to living systems, plasma processing of materials for microelectronic devices and other environmental remediation, and everyday lighting technology. Radiation damage to the DNA of living systems by ionizing radiation is predominantly initiated by dissociative attachment of secondary electrons to biological molecules and water. In spite of the importance of these fundamental processes, only fragments of the fundamental chemistry and physics are well understood, and only a few of the required cross sections and reaction rates for the multitude of important molecules are known with confidence.

Professor McCurdy's research group is developing new theoretical approaches and large-scale computational capabilities to attack these problems using the complex Kohn variational principle. Because the incident electron is indistinguishable from those of the target molecule, the

electronic structure of the molecule is not separable from the collision problem. New formalism is being coupled with the powerful existing technology of bound-state quantum chemistry to combine variational calculations on electronic collisions with a modern quantum chemistry program package. This work makes use of the tools of modern computer science, including new parallel algorithms appropriate for computers with thousands of processors. Multidimensional time-dependent methods are being used to treat the motion of nuclei during long-lasting electronic collisions near resonances corresponding to temporary negative ions.

Recently the long-standing problem of the complete quantum description of the collisional breakup of a quantum three-body system was effectively solved numerically for the first time by Professor McCurdy's group. The solution required a recasting of the Schrödinger equation in terms of complex valued coordinates for the electrons, thereby converting the complicated Coulomb boundary conditions for breakup into a simple form. To solve the resulting Schrödinger equation on a finite difference grid required extensive calculations using LBNL's massively parallel computers, even for a two-electron system.

Relevant Publications

http://jolt.lbl.gov/papers.html